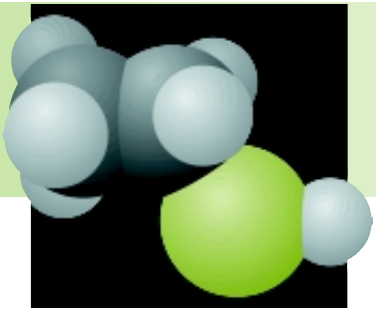
CHEMICALS

Project Fact Sheet



Mixed Solvent Corrosion

Benefits

- Estimated energy savings of 33 billion Btu per unit installed
- Reduces emissions of fly ash and particulate matter
- Improves plant safety
- Increases equipment life by 3 years
- Improves process simulation and estimation of the economics of new and existing chemical processes

Applications

The information and tools developed by this project will enable the U.S. chemical industry to reduce its expenses and energy loss due to corrosion. Improving the simulation of gas hydrate formation in upstream oil and gas applications makes these tools useful to the petroleum and forest products industry.

Prediction of corrosion in mixed solvents will reduce energy consumption

Corrosion is less predictable in ogranic or mixed-solvent environments than in aqueous solutions. This results in the over-design of equipment and the need for periodic equipment inspection in many chemical industry processes. Developing software products to predict corrosion of alloys in mixed solvent environments would save energy costs related to scheduled and unexpected shutdowns, increase productivity, and reduce the risk of environmental releases.

The commerical software package being developed will predict the stability of multicomponent alloys as well as thermodynamic equilibria, transport properties and rates of general corrosion in mixed solvent process environments. To accomplish these goals, project partners will expand and modify existing thermodynamic and kinetic modeling tools. While excellant electrochemical kinetic models have been available for decades, each one is system specific and almost all apply only to dilute solutions and were developed to address specfic questions. A broad based tool for predicting general corrosion for almost any chemical mixture operating between -50 and 300°C and 0 to 1500 bar would be useful to most chemical companies and could offer significant benefits within several other process industries.

Software Structure

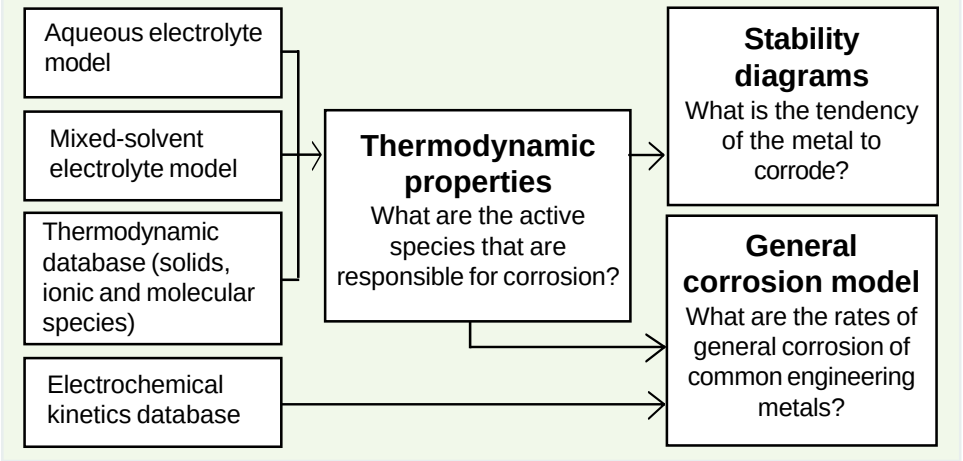


Diagram showing the structure of the software for simulating corrosion of engineering alloys in the chemical industry.

Project Description

Goal: Develop a set of comprehensive software tools that will enable the U.S. chemical industry to identify stable species and to predict the corrosion resistance of process equipment materials in commercial process environments.

These software tools will accurately predict the factors that are responsible for corrosion. In particular, they will predict:

1) The chemical composition, speciation, phase equilibria, component activities and transport properties of the bulk (aqueous, nonaqueous or mixed) phase that is in contact with the metal.
2) The phase equilibria and component activities of the alloy phase(s) that may be subject to corrosion.
3) The interfacial phenomena that are responsible for corrosion at the metal/solution or passibe/solution interface.

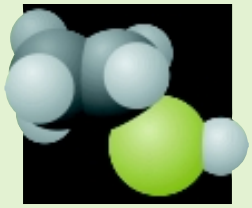
Progress and Milestones

Project research will focus on the following areas:

- Determine the activity of alloy components and review the basis of the model for developing stability diagrams
- Identify critical mixed-solvent environments
- Develop a thermodynamic model for mixed-solvent electrolyte systems
- Incorporate alloy model into stability diagrams. Verify and commericialize the diagrams
- Integrate the mixed-solvent model with OLI software
- Develop an electrochemical model for simulating rates of general corrosion
- Extend transport property models to mixed-solvent systems
- Integrate the mixed-solvent model with stability diagrams
- Verify and commercialize software for generating stability diagrams for mixed-solvent systems
- Verify the kinetic model and commercialize the software products

Commercialization

OLI Systems intends to commercialize the software tools once they have been developed and verified. OLI Systems is currently working with major chemical companies and has experience in developing and commercializing software for the chemical industry. After release of the new software tools, project partners will conduct a symposium to introduce the new product.



Project Partners

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